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High temperature thermodynamic, mechanical and kinetic properties from first principles

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Predicting high temperature thermodynamic and kinetic properties of technologically important materials from first principles remains a major challenge. Most materials of practical interest are multi-component and exhibit varying degrees of long and short-range order. In addition to configurational disorder, anharmonic vibrational excitations can also be important in determining high temperature thermodynamic properties and must be accounted for in the description of a subset of structural phase transitions. The complexity of solid-state diffusion also increases with the number of components in the solid. Effective Hamiltonians parameterized from first principles allow for a systematic treatment of relevant excitations within statistical mechanical predictions of finite temperature thermodynamic, mechanical and kinetic properties of solids. In this talk we will illustrate this approach as applied to a variety of technologically important alloys.